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# HYDRODYNAMIC AND ENERGY-TRANSPORT MODELS FOR SEMICONDUCTOR DEVICE SIMULATION: EXTENSIONS AND CRITICAL ISSUES*



**Разом зі статтею [1] ми надаємо детальний перегляд основних транспортних моделей. Також ми наводимо розширення основних моделей і пробуємо пролити додаткове світло на особливо критичні аспекти, що асоціюються з цими транспортними моделями.**

**In a com-panion paper [1] we gave a detailed review of the basic transport models. Here we present extensions to the basic models and try to shed some additional light on the critical issues associated with these transport models.**

## 1 Introduction

As the size of state-of-the-art devices is continually reduced, non-local behavior becomes a critical issue in the simulation of these structures. The well established drift-diffusion (DD) model [2] which is still predominantly used by engineers around the world cannot cover these effects as the electron gas is assumed to be in thermal equilibrium with the lattice temperature. To overcome this limitation, hydrodynamic and energy transport models have been published, first by Stratton [3] and by Bløtekjær [4]. Both models were derived assuming parabolic bands and homogeneous materials and are discussed in detail in [1]. As the assumption of parabolic bands and homogeneous materials limits the validity of the models, several extensions have been proposed which will be covered in detail here. Furthermore, even for the basic models some simplifying assumptions had to be made to yield models suitable for engineering purposes. In the following we review some of these assumptions and the implications for practical device simulation.

## 2 Non-Parabolicity Extensions

The general hydrodynamic equations given in [1] are valid for any band structure as $\mathbf{F}$ depends only on the spatial gradient of the dispersion relation. However, parabolicity assumptions are invoked to derive the closure relations for the momentum and the average energy. On the other hand, non-parabolicity effects enter the HD equations through the models used for the collision terms. A good example is the mobility whose homogeneous values are frequently obtained through measured $\mathbf{v}(\mathbf{E})$ characteristics. This mobility contains the full information of a real band structure, something which is much more difficult to obtain with MC simulations where

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band structure, something which is much more difficult to obtain with MC simulations where the mobility has to be modeled using microscopic scattering rates [5]. As pointed out in the discussion of the average energy, there is no analytic relationship between $\langle \mathcal{E} \rangle$ and $\mathbf{v}$ in the general case. For parabolic bands the carrier temperature is normally defined via the average carrier energy as

$$T_n = \frac{2}{3k_B}\left(\langle \mathcal{E} \rangle - \frac{m^* \mathbf{v}^2}{2}\right) \tag{1}$$

Unfortunately, there is no similar equation for non-parabolic bands. Another possibility is to define the temperature via the variance of the velocity as [6]

$$T^* = \frac{m^*}{3k_B}\langle \mathbf{u}^2 \rangle \tag{2}$$

Definitions (1) and (2) are consistent with the thermodynamic definition of the carrier temperature in thermodynamic equilibrium and both are identical for non-equilibrium cases when a constant carrier mass is assumed which in turn corresponds to the assumption of parabolic energy bands. However, large differences are observed when a more realistic band structure is considered [6, 7].

## 2.1 The Generalized Hydrodynamic Model

Thoma *et al.* [6, 7] proposed a model which they termed 'generalized hydrodynamic model'. Instead of using the average energy *and* the temperature as variables in their formulation, they opted for a temperature-only description. To obtain a form similar to standard models, they defined the temperature according to (2) which differs significantly from (1) for non-parabolic bands. Instead of the momentum weight functions $\hbar\mathbf{k}$ and $\hbar\mathbf{k}\mathcal{E}$, they used $\mathbf{u}$ and $\mathbf{u}\mathcal{E}$ to derive the moment equations of order one and three. Without assuming a Kane dispersion they derived the following equations for the current and energy flux density

$$\mathbf{J} = \frac{\tau_i}{\tau_i^*}\mu^* k_B \nabla(nT^*) + q\mu^* n\mathbf{E} \tag{3}$$

$$\nabla \cdot (n\mathbf{S}) = -\frac{3k_B}{2}\partial_t(nT^*) + \mathbf{E}\cdot\mathbf{J} - n\frac{3k_B}{2}\frac{T^* - T_L}{\tau_\mathcal{E}^*} \tag{4}$$

$$n\mathbf{S} = -\frac{\mu_S^*}{\mu^*}\frac{5}{2}\frac{k_B T^*}{q}\left(\mathbf{J} + \mu^*\frac{\tau_i}{\tau_i^*}nk_B\nabla T^*\right) \tag{5}$$

All relaxation times and mobilities are modeled as a function of $T^*$ and explicit formulas were given in [8]. The advantage of this formulation is that it can be applied to arbitrary band structures. Thoma *et al.*, however, used parameters extracted from MC simulations employing the Kane dispersion relation.

## 2.2 Model of Bordelon

Another non-parabolic formulation was derived by Bordelon *et al.* [9, 10] which explicitly assumed a Kane dispersion. They used the weight functions $1$, $\hbar\mathbf{k}$ and $\mathcal{E}$ and closed the system by ignoring the heat flux. To avoid the problem with the missing energy-temperature relation, they formulate their equation system solely in $w$. By introducing the function $H(w) =$

$(1+\alpha w)/(1+2\alpha w)$ in the approximation for $\hat{\mathrm{U}}$ [11] they obtain

$$\mathbf{J} = \mu\frac{2}{3}\nabla(nwH(w)) + \mathrm{q}\mu n\mathbf{E} \qquad n\mathbf{S} = -\Omega(w)w\frac{\mathbf{J}}{\mathrm{q}} \tag{6}$$

with $\Omega(w) \approx 1.3$. In the comparison made by Ramaswamy and Tang [11] the predicted $\mathbf{v}$ and $\mathbf{S}$ curves agree quite well with the MC data, even with this simplified model for $\mathbf{S}$.

## 2.3 Model of Chen

In [12] Chen *et al.* published a model which they termed 'energy transport model'. They tried to include non-parabolic and non-Maxwellian effects to a first order. Their approach is based on Stratton's model and the use of Kane's dispersion relation. Their Ansatz contains a non-Maxwellian factor $\gamma$ which, however, does not show up in the final equations which read

$$\mathbf{J} = \mathrm{k_B}\nabla(n\mu T_n) + \mathrm{q}\mu n\mathbf{E} \qquad n\mathbf{S} = -C_e\Big(\mu n\mathrm{k_B}T_n\mathbf{E} + \frac{\mathrm{k_B^2}}{\mathrm{q}}\nabla(n\mu T_n^2)\Big) \tag{7}$$

with

$$C_e = \Big(\frac{5}{2} - p\Big)\Big(1 - \frac{\mathrm{k_B}\alpha T_n}{2}\Big) \qquad \langle\mathcal{E}\rangle = \Big(1 + \frac{5}{2}\alpha\mathrm{k_B}\mathrm{T_n}\Big)\frac{3}{2}\mathrm{k_B}T_n \tag{8}$$

Sadovnikov and Roulston [8] showed that Chen's model fails to predict proper velocity profiles and is not consistent with homogeneous simulation results.

## 2.4 Model of Tang

Tang *et al.* [13] gave very elaborate expressions for $\hat{\mathrm{U}}$, $\mathbf{p}$ and $\hat{\mathrm{R}}$ to close the equation system. Their discussion aims at a correct handling of the inhomogeneity effects normally ignored. By observing that $(\hat{\mathrm{U}} - \mathbf{v}\otimes\mathbf{p})$ and $(\hat{\mathrm{R}} + 2.5w\mathbf{v}\otimes\mathbf{p})$ show nearly no hysteresis for an $n^+$-$n$-$n^+$ test-structure they proposed the following closure relations

$$\hat{\mathrm{U}} = \frac{2}{3}w\hat{\mathrm{I}} + \mathbf{v}\otimes\mathbf{p} + u(w)\hat{\mathrm{I}} \qquad \hat{\mathrm{R}} = \frac{10}{9}w^2\hat{\mathrm{I}} - 2.5w\mathbf{v}\otimes\mathbf{p} + r(w)\hat{\mathrm{I}} \tag{9}$$

$$\mathbf{p} = m^*\mathbf{v} + 2\alpha m^*\mathbf{S} \tag{10}$$

with $u(w)$ and $r(w)$ being single-valued fit-functions. They used a Kane dispersion for the MC simulation which might somehow limit the validity of the expressions above. Unfortunately, the additional convective terms are likely to cause numerical problems in an actual multi-dimensional implementation.

## 2.5 Model of Smith

In [14] Smith and Brennan derived two non-parabolic equation sets for inhomogeneous and degenerate semiconductors (see also [15, 16]). They used both the Kane dispersion and a simpler power-law approximation after Cassi and Riccò [17] because the Kane dispersion relation cannot be integrated analytically. They showed that the typically employed binomial expansion of the Kane-integrands looses its validity and physically not consistent results are obtained. The power-law approximation, on the other hand, approaches the parabolic limit and has a larger range of validity.

### 2.6 Model of Anile

Anile and Romano [18] and Muscato [19] derived expressions for the closure $\hat{\mathrm{U}}$ and $\hat{\mathrm{R}}$ using the maximum entropy principle. In addition, they were able to derive expressions for the collision terms. They found that their model fulfills Onsagers reciprocity principle and gave a comparison with other hydrodynamic models.

### 2.7 Comparison

A comparison of the simple ET model with the expressions given by Thoma *et al.*, Lee *et al.*, Chen *et al.*, and Tang *et al.* for Si bipolar transistors is given by Sadovnikov and Roulston [8] who observed no significant differences in the simulated output characteristics.

## 3 Extensions for Semiconductor Alloys

The derivations given above are restricted to homogeneous materials where the effective carrier masses and the band edge energies do not depend on position. Over the last years extensive research has been made concerning III-V materials and SiGe heterostructure devices. Especially for III-V materials inclusion of the carrier temperature in the transport equations is considered a must. State-of-the-art III-V heterostructure transistors employ many different combinations of materials. In addition differently graded profiles have been used. SiGe bipolar transistors with graded Ge profiles in the base have also been widely investigated. To properly account for the additional driving forces due to changes in the effective masses and the band edge energies the energy-transport models have been extended accordingly. The foundation for these extensions was laid in the pioneering work by Marshak for the drift-diffusion equations [20, 21]. These concepts have been applied to the energy-transport models by Azoff in [22, 23, 24]. In the case of a position-dependent parabolic band structure, the force exerted on an electron is given as

$$\mathbf{F} = -\nabla E_c + \mathcal{E}\frac{\nabla m^*}{m^*} \tag{11}$$

These additional forces give rise to an additional component in the current relation and the electric field is replaced by an effective electric field which also contains the gradient of the band edges.

$$\mathbf{J} = \mu n \nabla E_c + \frac{2}{3}\mu\nabla(nw) - \mu n w \nabla \ln(m^*) \qquad \mathbf{S} = -\frac{5}{3}\frac{\mathbf{J}w}{q} - \frac{10}{9}\mu k_B n w \nabla w \tag{12}$$

An extension to non-parabolic bandstructures has been presented by Smith *et al.* [14, 15].

## 4 Multiple Band Models

Bløtekjær's [4] equations were originally devised for semiconductors with multiple bands. Woolard *et al.* [25, 26] extended these expressions for multiple non-parabolic bands in GaAs. Other GaAs models can be found in [27, 28]. Wilson [29] gave an alternate form of the hydrodynamic model which he claims to be more accurate than [4]. Another multivalley non-parabolic energy-transport model was proposed in [30].

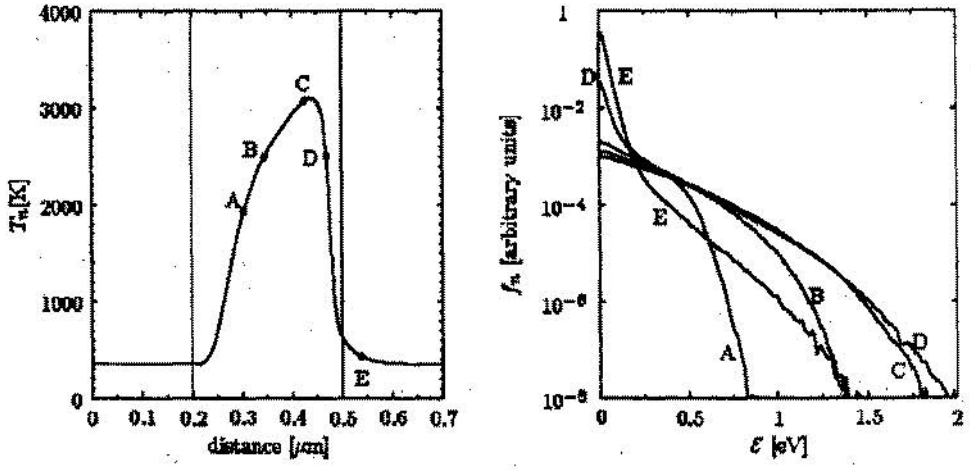


Figure 1: Electron temperature and distribution function five characteristics points inside the $n^+$-$n$-$n^+$ test-structure. Note that the average energies at the points B and D are the same.

# 5 Band Splitting Models

As device geometries are further reduced without according reduction of the supply voltages, the electric fields occurring inside the devices increase rapidly. Furthermore, strong gradients in the electric field are observed. These highly non-homogeneous field distributions give rise to distribution functions which deviate significantly from the frequently assumed Maxwellian distribution. Furthermore, as has been pointed out in [31], the distribution function is not uniquely described using just the average carrier energy. This is depicted in Fig. 1 which shows some electron distribution functions inside an $n^+$-$n$-$n^+$ test-structure obtained by MC simulation. Points ABC are in the channel while the points D and E are taken from the drain region. In the drain region, the overpopulation of the high-energy tail is obvious, whereas in the channel it is underpopulated, showing a significant thermal tail [32].

Several moment based models have been proposed so far which aim at obtaining some additional information about the DF to the average energy. One approach is to split the energy range at some characteristic energy and handle both energy ranges with a two-population and two-temperature model [33, 34]. As these models were aimed at modeling impact ionization the band gap energy was taken as the characteristic energy. This approach leads to various additional macroscopic parameters which model the transitions between the two energy regions. Determination of these parameters relies on carefully set up MC simulations. Due to this specialization to impact ionization, this model would have to be reformulated if another energy range is of interest as is the case for the calculation of gate currents. Thus this approach is difficult to generalize if both effects need to be captured at the same time which is demanded for state-of-the-art devices. A special formulation using two electron populations has been proposed in [35] for those regions where the high-energy tail is heavily populated. In [36] Tang gave a simplified version of the two energy model [33] which used assumptions similar to those made by Cook and Frey [37].

# 6 Electro-Thermal Extensions

One of the problems resulting from the reduction in device geometries is that the generated heat has to be kept to a minimum. To capture these self-heating effects, the moment equations have to be extended to account for non-constant lattice temperature. A detailed treatment of this subject was given by Wachutka [38] for the classical DD equations. Chen *et al.* gave an extension for the energy-transport models in [39]. Benvenuti *et al.* introduced a thermal-fully hydrodynamic model in [40]. A detailed discussion can be found in [41].

# 7 Critical Issues

The models given above employ various approximations of different severity. As these approximations have been discussed extensively in literature, they will be summarized in the following sections.

## 7.1 Closure

The method of moments transforms the BTE into an equivalent, infinite set of equations. One of the severest approximation is the truncation to a finite number of equations (normally three or four). The equation of highest order contains the moment of the next order which has to be suitably approximated using available information, typically the lower order moments. Even though no form of the distribution function needs to be assumed in the derivation, an implicit coupling of the highest order moment and the lower order moments is enforced by this closure. For their generalized HD model, Thoma *et al.* [6, 7] give a maximum error of 30% which can be quite significant. One approach to derive a suitable closure relation is to assume a distribution function and calculate the fourth order moment. Geurts [42] expanded the distribution function around drifted and heated Maxwellian distribution using Hermite polynomials. This gives a closure relation which generalizes the standard Maxwellian closure. However, these closures proved to be numerically unstable for higher electric fields. Liotta and Struchtrup [43] investigated a closure using an equilibrium Maxwellian which proved to be numerically very efficient but with unacceptable errors for higher electric fields. For a discussion on heated Fermi-Dirac distributions see [14, 16]. Ramaswamy and Tang [11] gave a comparison of different closure relations available in literature.

## 7.2 Tensor Quantities

An issue which has only been vaguely dealt with is the approximation of the tensors by scalar quantities, such as the carrier mass and the carrier temperature. One-dimensional simulations have been carried out in [44] which indicate that the longitudinal temperature component $T_l$ is larger than the transverse temperature component $T_t$, indicating that the distribution function is elongated along the field direction and thus that the normally assumed equipartition of the energy is invalid. A rigorous approach has been taken by Pejčinović *et al.* [45] who model four components of the temperature tensor. They observed no significant difference between the scalar temperature and $\mathrm{tr}\,(\bar{\bar{T}}_n)/3$ for ballistic diodes and bipolar transistors but a 15 % difference for aggressively scaled MOSFETs in the linear region of the transfer characteristics. Tang *et al.* [13] observed that the energy tensor is not a single valued function of the average energy and give models using available moments (see (9)).

## 7.3 Drift Energy vs. Thermal Energy

Another common approximation is the neglection of the drift energy in the average carrier energy [37]

$$w = \frac{m v^2}{2} + \frac{3}{2} k_B T_n \approx \frac{3}{2} k_B T_n \qquad (13)$$

As has been pointed out by Baccarani and Wordeman [46], the convective energy can reach values comparable to thermal energy. A plot of the difference of these temperature definitions inside an $n^+$-$n$-$n^+$ test-structure is given in Fig. 2. As can be seen, the error introduced by this approximation is larger than 15 % in the beginning of the channel where the carrier temperature is still low and a velocity overshoot is observed. This effect has been studied in [47].

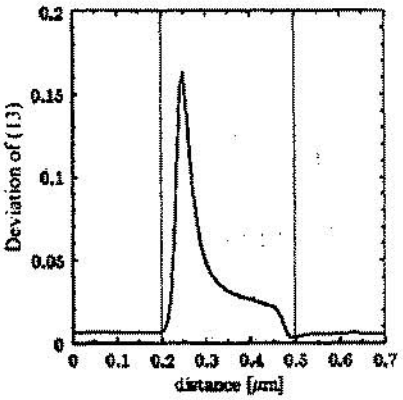


Figure 2: Effect of approximation (13) on the carrier temperature and the deviation introduced by it obtained by a MC simulation of the $n^+$-$n$-$n^+$ test-structure.

## 7.4 Relaxation Times

The relaxation times have traditionally been derived from homogeneous field measurements or MC simulations. For homogeneous fields, there is a unique relationship between the electric field and the carrier temperature via the local energy balance equation which can be used as a definition for $\tau_\varepsilon$. However, due to the modeling of the collision terms, the relaxation times depend on the distribution function. Since the distribution function is not uniquely described by the average energy, models based on the average energy are bound to fail. Furthermore, the band structure plays a dominant role. Nevertheless, all models should be able to correctly reproduce the homogeneous limit. In the following, some models for Si are reviewed.

### 7.4.1 Mobility

Two models for the energy dependence of the mobility are frequently used, the model after Baccarani *et al.* [46, 48]

$$\frac{\mu(T_n)}{\mu_0} = \frac{T_L}{T_n} \qquad (14)$$

and the model after Hänsch [49, 50]

$$\frac{\mu(T_n)}{\mu_0} = \left(1 - \frac{3}{2}\frac{\mu_0}{\tau_\varepsilon v_s^2}\left(\frac{k_B T_L}{q} + \frac{2}{5}\frac{nS}{J}\right)\right)^{-1} \qquad (15)$$

For homogeneous materials $S/J = 5k_B T_n/(2q)$ which can be used to simplify (15) as

$$\frac{\mu(T_n)}{\mu_0} = \left(1 + \frac{3}{2}\frac{\mu_0 k_B}{q\tau_\varepsilon v_s^2}\left(T_n - T_L\right)\right)^{-1} \qquad (16)$$

As has been shown in [44, 51] expression (16) reproduces the mobility quite well in the regions with increasing $\mathbf{E}$. However, for decreasing $\mathbf{E}$ (15) should be used [44, 52].

Tang *et al.* [13] proposed another expression by separating the homogeneous from the inhomogeneous part of the mobility. They suggest to model the collision term $\mathbf{C}_p$ as

$$n\mathbf{C}_p = \frac{\mathbf{J}}{\mu} = \frac{\mathbf{J}}{\mu^*} + \lambda_p n \nabla \cdot \hat{\mathbf{U}} \tag{17}$$

with $\mu^*$ being the homogeneous mobility. The second term of (17) can then be moved to the left-hand-side of the current relation to give a Stratton-like energy gradient expression $(1-\lambda_p)n\nabla\hat{U}$. The quantity $\lambda_p$ has been extracted from MC simulations as

$$\lambda_p = \begin{cases} 0.15 & \text{for} \quad \nabla\hat{U} > 0 \\ 0.50 & \text{for} \quad \nabla\hat{U} < 0 \end{cases} \tag{18}$$

In [53] Tang *et al.* give an improved expression.

### 7.4.2 Energy Relaxation Time

The simplest approach at modeling $\tau_\mathcal{E}$ a constant approximation with values in the range 0.3 – 0.4 ps. Baccarani *et al.* [48, 46] proposed the expression

$$\tau_\mathcal{E}(T_n) = \frac{3}{2}\frac{k_B\mu_0}{qv_s^2}\frac{T_nT_L}{T_n+T_L} + \frac{m^*\mu_0}{2q}\frac{T_n}{T_L} \tag{19}$$

Note that when

$$\tau_\mathcal{E} = \frac{3k_B\mu_0 T_L}{2qv_s^2} \tag{20}$$

is used in the Hänsch mobility model [49], the Baccarani and Hänsch models are equivalent in the homogeneous case [54]. It is also to note that (14) should be used together with (19) whereas in the Hänsch approach $\tau_\mathcal{E}$ is only required to be independent of the temperature for (15) to correctly predict the homogeneous limit. A comparison of these two models is given in Fig. 4 where the differences for the non-homogeneous case are visible. A discussion of the inconsistencies resulting from mixing arbitrary energy-dependent mobility and energy relaxation time models can be found in [55].

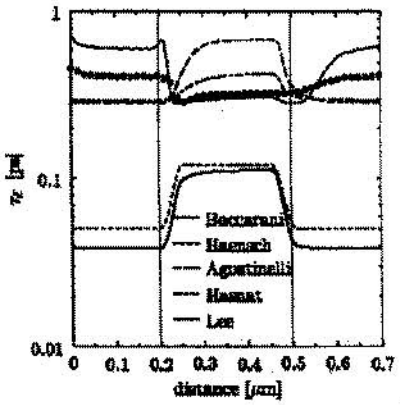


Figure 3: Comparison of different energy relaxation time models for a $n^+$-$n$-$n^+$ test-structure. The open circles are from a MC simulation.

Agostinelli *et al.* [56] proposed a model which is fit to the data of Fischetti [57]

$$\frac{\tau_\mathcal{E}(W)}{1\text{ ps}} = \begin{cases} 0.172 + 2.656W - 3.448W^2 & \text{for } W \le 0.4 \\ 0.68 & \text{for } W > 0.4 \end{cases} \tag{21}$$

with $W = w/(1\text{eV})$. Another more elaborate fit to the data of Fischetti is given in [58]. A maximum value of 0.68 ps seems to be too high, and yet another fit to newer data from Fischetti has been published by Hasnat *et al.* [59] as

$$\frac{\tau_\mathcal{E}(W)}{1\text{ ps}} = 0.27 + 0.62W - 0.63W^2 + 0.13W^3 + 0.01W^4 \tag{22}$$

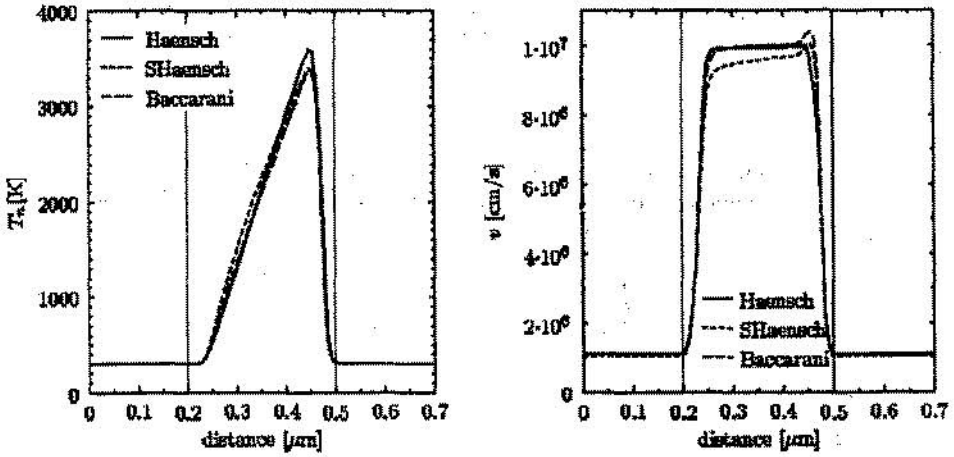


Figure 4: Electron temperature and velocity distribution inside the $n^+$-$n$-$n^+$ test-structure. $\mu$ and $\tau_\mathcal{E}$ were modeled according to (15)+(20) and (14)+(19). SHaensch stands for the simplified Hänsch model (16).

with a maximum value of approximately 0.42 ps. Another expression was given by Lee and Tang [44] as

$$\tau_\mathcal{E}(w) = t_0 + t_1\eta(w) + t_2\exp(-\beta\eta(w)) \tag{23}$$

with $\eta = w/w_0 - 1$ and the parameters $t_0 = 0.28$ ps, $t_1 = 3$ fs, $t_2 = 2.2$ ps, and $\beta = 10$.

A comparison for these energy relaxation time models is given in Fig. 3 where the differences between the models is obvious. Also shown is the result of our MC simulation. Note that for the Baccarani and Hänsch models the low-field mobility has been calculated with the expression of Caughey and Thomas [60] using the given doping profile and $v_s = 10^7$ cm/s. The other models offer no adjustment of the low-field mobility which can be considered a serious drawback and a cause for inconsistencies. A detailed comparison of the effects of both relaxation times and transport models on the performance of Si bipolar transistors is given in [8].

As the temperature profile occurring inside the device is very sensitive to $\tau_\mathcal{E}$ this disagreement is rather astonishing and further research on this topic is in order.

### 7.4.3 Energy Flux Relaxation Time

The ratio of the energy flux mobility and the mobility $\tau_\mathcal{S}/\tau_p$ is usually modeled as a constant with values in the range 0.79-1 [44, 13]. Tang *et al.* [13] proposed an expression in analogy to (17) by separating the homogeneous and inhomogeneous parts. They suggest to model the collision term $\mathbf{C}_{p\mathcal{E}}$ as

$$\mathbf{C}_{p\mathcal{E}} = -\frac{q\mathbf{S}}{\mu_\mathcal{S}^*} + \lambda_{p\mathcal{E}}\nabla\cdot\hat{\mathbf{R}} \tag{24}$$

with $\mu_S^*$ being the homogeneous energy flux mobility. Expressions for $\mu_S^*$ and $\lambda_{\mu\mathcal{E}}$ can be found in [13].

### 7.5 Spurious Velocity Overshoot

Models based on Bløtekjær's approach have been frequently associated with spurious velocity overshoot (SVO), that is, non plausible spikes in the velocity characteristics which do not occur in MC simulations. This effect can be seen in Fig. 4 where the SVO is clearly visible. Several theories have been put forward to explain this effect. Some authors argue that it is related to the hysteresis in the mobility [31], whereas others relate it to non-parabolicity effects [9]. Still others argue that it is related to the closure of the energy-transport equation system [47]. The improvement obtained by the non-parabolic model [9] is probably due to the improved closure relation for $\hat{\mathbf{R}}$. As already argued by [47], SVO is not likely to be caused only by the mobility because the mobility is not properly modeled in the whole $\nabla \cdot \hat{\mathbf{U}} < 0$ region and SVO is restricted to a very small area. Lee and Tang [44] investigated SVO using different mobility models and found that improvement is possible when proper mobility models are used. For example, with the Hänsch mobility model (15) these spikes are strongly diminished but not completely removed. Unfortunately, our own MC simulations show that (15) also overestimates the real velocity overshoot at the beginning of the channel. Chen *et al.* [61] proposed a model based on Stratton's approach. In their simplified analysis they used Baccarani's mobility model which thus removes any thermal diffusion current inside the whole device which is definitely not physically sound [13].

## 8 Validity of Moment Based Models

When the critical dimensions of devices shrink below a certain value (around 100 nm for Si at room temperature) MC simulations reveal strong off-equilibrium transport effects such as velocity overshoot and quasi-ballistic transport. So the range of validity for moment based models has been extensively examined. Furthermore, with shrinking device geometries quantum effects gain more importance and limit the validity for the BTE itself [62]. Banoo and Lundstrom [63] compared the results obtained by an energy-transport model with a DD model and a solution of the BTE obtained by using the scattering matrix approach. They found that this energy-transport model dramatically overestimates both the drain current and the velocity inside the device. Tomizawa *et al.* [64] found through a comparison with MC simulations that relaxation time based models tend to overestimate non-stationary carrier dynamics, especially the energy distribution. Nekovee *et al.* [65] compared moment hierarchy based models with a solution of the BTE and found that moment based models fail in the prediction of ballistic diodes because the moment hierarchy converges to slowly. A similar conclusion was drawn by Liotta and Struchtrup [43] who found that a hierarchy containing 12 moment equations was needed to reproduce results similar to those obtained by spherical harmonics expansions.

## 9 Simplified Models

Despite of the limitations and approximations contained in the moment equations given above, the solution procedure can be quite involved. Thus several authors tried to find suitable approximations to simplify the analysis. These approximations were frequently used in post-processors to account for an average energy distribution different from the local approximation. Slotboom

*et al.* [66] used this technique to calculate energy-dependent impact ionization rates via a post-processing model. Cook and Frey [37, 67] proposed a simplified model by using the approximations $v_x \gg v_y$ and $E_x \gg E_y$ in a two-dimensional Si MESFET to yield

$$\frac{\partial w}{\partial x} = \frac{21}{20} q E_x - \frac{9}{20}\left(\frac{40\, m^*(w - w_0)}{9\, v_x \tau_E \tau_p} + q^2 E_x^2\right)^{1/2} \tag{25}$$

Thus, the energy balance equation and the continuity equation become decoupled and the complexity of the problem is considerably reduced. Approximations for GaAs were also given. Although these approximations might have delivered promising results, progress in the size-reduction of state-of-the-art devices makes the assumptions $v_x \gg v_y$ and $E_x \gg E_y$ questionable. In particular, for deep-submicron MOSFETs, velocity overshoot influences the electric field distribution for a given bias condition, and effectively defines a higher drain saturation voltage which in turn defines a higher current [68].

To bring the energy-transport equations into a self-adjoint form Lin *et al.* [69] approximated the carrier temperature in the diffusion coefficient by the lattice temperature as

$$\mathbf{J} = \mu k_B \underbrace{T_n}_{\approx T_L} \nabla n + \mu k_B n \nabla T_n + q n \mu \mathbf{E} \tag{26}$$

which will underestimate the diffusion current by a factor of $\approx 10-20$ for state-of-the-art devices and can therefore not be recommended.

# 10 Conclusions

The uncertainties introduced by the approximation of the collision terms pose a bib problem to the accuracy of the hydrodynamic models. They are modeled via relaxation times and mobility models. Expression for these are normally extracted from homogeneous MC simulations. As has been clearly shown, homogeneous MC simulation data are not sufficient for the simulation of state-of-the-art devices as neither the relation times nor the closure relations are single-valued functions of the average energy. This used to be one of the advantages of the macroscopic transport models over the MC method because measured $\mu(E)$ characteristics could be directly incorporated into the simulation which is not possible for the microscopic approach taken in the MC method. Unfortunately, data for inhomogeneous situations are difficult to extract from measurements due to the complex interaction between the various parameters. Therefore, MC simulations of $n^+$-$n$-$n^+$ test-structure were performed to extract the desired data.

Another critical issue is due to the closure relations introduced to reduce the number of unknowns. Several extensions for non-parabolic bands have been reviewed, which, due to the nature of the problem, can only give an approximate solution to the problem.

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